

Isopropyl carbamate
1746-77-6 | DTXSID9051795

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.29e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.70e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

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Propyl carbamate

Measured: 7.41e-01

Predicted: 1.25

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Acrylamide

Measured: 9.00

Predicted: 9.79

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2-Fluoroacetamide

Measured: 13.0

Predicted: 12.6

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Emylcamate

Measured: 2.75e-02

Predicted: 3.90e-02